N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine

3089-11-0 | DTXSID9027520

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.18e-02 mol/L

Global applicability domain: Outside

Local applicability domain index: 2.54e-01

Confidence level: 3.27e-01

Nearest Neighbors from the Training Set

Image not found
Dimorpholamine
Measured: 1.25
Predicted: 2.53e-01

Image not found
Propentofylline
Measured: 1.04e-01
Predicted: 1.65e-02

Image not found
Benomyl
Measured: 1.31e-05
Predicted: 3.43e-03

Image not found
Pentoxifylline
Measured: 2.77e-01
Predicted: 8.87e-02

Image not found
2,4-Bis((3-methoxypropyl)amino)-6(methylthio)-s-triazine
Measured: 3.32e-04
Predicted: 1.23e-02